

Syllabus for CHEM 453L: *Biomolecular Structure & Function Lab* – Fall 2020
Coastal Carolina University
Version 12 November 2019

Instructor: Brian Lee, Ph.D. **Email:** brianlee@coastal.edu
Office Hours: 9⁰⁰ – 10⁰⁰ am MWF **Office:** Science II 301-C
Practical: 11⁰⁰ am-1⁵⁰ pm Tuesdays in Smith Science 208

Required Laboratory Workbook:

The PyRosetta Interactive Platform for Protein Structure Prediction and Design: A Set of Educational Modules, Johns Hopkins University, Baltimore, MD, 2016. ISBN13: 978-1542402132
by Jeffrey J. Gray, Sidhartha Chaudhury, Sergey Lyskov, and Jason Labonte.

Biochemistry Texts on Reserved in Kimbel Library:

Biochemistry, 3rd Ed., Voet & Voet, QP514.2.V64 2004
Biochemistry, 6th Ed., Berg, Tymoczko & Stryer, QP514.2.S66 2007
Fundamentals of Biochemistry, 2nd Ed., Voet, Voet & Pratt QD 415.V63 2006
Protein Structure and Function, Petsko & Ringe QP551.P48 2004

Prerequisite: *General Organic Chemistry* (CHEM 331/331L/332/332L) and *Calculus* (MATH 160)

Pre/Co-requisites: *Physics* (PHYS 205 or PHYS 211)

Co-requisite: *Biomolecular Structure & Function Lab* (CHEM 453L)

Course Description: The practical laboratory course will introduce students to methods in structural biology that focus on the study of proteins and nucleic acids. Computational methods will include comparative sequence analysis, ab initio and comparative molecular modeling, molecular dynamics simulations, and structure calculations based on experimental data. Experimental studies will be assessed to demonstrate correlations between functional activity and the structural features of biomolecules.

Course Objectives: Students should develop knowledge and skills in the following areas:

1. molecular graphics for visualizing and measuring biomolecular structures
2. molecular modeling for structure prediction and engineering applications
3. correlations between structure and function based on biophysical studies

Student Learning Outcomes: Students will show proficiency in the following techniques:

1. visualize and manipulate biomolecular structures in three dimensions.
2. create graphics for presentation that highlight functionally significant features.
3. use computational approaches to measurements of stability and dynamics.
4. visualize active site features that play a role in enzyme reaction mechanisms.
5. visualize biomolecular surfaces and identify potential intermolecular binding sites.
6. create models of biomolecules with ab initio and homology modeling techniques.
7. analyze structural data to extract parameters and restraints for structure determination.
8. calculate experimental structures using geometric and molecular dynamics methods.
9. assess biophysical studies to identify functionally significant structural features.

Course Requirements: Twelve lab projects will be developed during the lab sessions. Some lab projects will be completed in-class. Other projects may require additional work or span multiple lab sessions. If projects are not completed in-class, then assignments are due before the next lab session.

Grading Scale:	A 1000–900 pts	B ⁺ 899–870 pts	B 869–800 pts	C ⁺ 799-770 pts
	C 769–700 pts	D ⁺ 699-670 pts	D 699–600	F 599–0 pts

Grading Policy: Your final grade will be based on exams and quizzes, as follows:

4 small projects (50 points each) =	200 maximum points =	20 %
<u>8 large projects (100 points each) =</u>	<u>800 maximum points =</u>	<u>80 %</u>
Total =	1000 maximum points =	100 %

Academic Integrity Code: Coastal Carolina University is an academic community that expects the highest standards of honesty, integrity and personal responsibility. Members of this community are accountable for their actions and reporting the inappropriate action of others and are committed to creating an atmosphere of mutual respect and trust. In accordance with the Code of Student Conduct and your Honor Pledge, plagiarism, cheating, attempted cheating and all other forms of academic dishonesty will not be tolerated. Any student caught cheating on an exam will automatically receive zero points for that exam, which cannot be dropped from the final grade.

Class Attendance Policy: You are obligated to attend class regularly. The instructor is required to report attendance to the Financial Aid Office in compliance with Title IV of the Higher Education Act of 1965 and University Policies. Absences, excused or not, do not absolve you from the responsibility of completing all assigned work promptly. Excused absences must be approved beforehand (emergencies excepted). Accommodations for excused absences may be made at the discretion of the instructor.

Class Etiquette: Please, if you must arrive late or leave early, do not disrupt the class. Turn off your cell phone ringer during the class. Eating, texting, gaming, web browsing or reading a newspaper is not permitted during class. Use of a laptop, tablet or smartphone for taking notes and referencing course material is permitted as long as there is no disruption to the class. Please be polite in all discussions in class and respectfully of others. Questions and discussions are encouraged and expected in class. You are encouraged to work together and help each other understand the course material. Study groups are encouraged.

Accommodations for Students: Coastal Carolina University, in accordance with the Americans with Disabilities Act Amendments Act of 2008 (ADAAA) and Section 504 of the Federal Rehabilitation Act of 1973, will provide reasonable accommodations for eligible students with disabilities. If you require special assistance, please see me privately and seek assistance directly from the Office of Accessibility and Disability Services (843-349-2503 or www.coastal.edu/disabilityservices/). You are responsible for initiating arrangements of accommodations for tests and other assignments in collaboration with the Office of Accessibility and Disability Services and your professors.

Contingency Class Time: In the event of hazardous weather, faculty, staff, and students are requested to listen to local radio and television stations, or visit the Coastal Carolina University website for official closing announcements. If normal class activities are disrupted due to illness, emergency, inclement weather, or crisis situation, the syllabus, class schedule and course requirements may be modified to allow completion of the course. Changes may include the additional class meeting times.

Changes and Amendments: The syllabus, class schedule and course requirements are subject to change by the instructor with notice to the student as the semester progresses. All changes will be posted.

Schedule for CHEM 453L: *Biomolecular Structure & Function Lab* – Fall 2018
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Textbook: *PyRosetta*, by Gray, Chaudhury, Lyskov & Labonte (2016)

Tentative Class Schedule:

Date	Topic	
Aug 25	Introduction to Biomolecular Structure and Function	
Sep 1	Lab 1: Bioinformatics and Nucleic Acid Structure	50 pts
8	Lab 2: Eterna: RNA Folding Game (Rosetta based)	100 pts
15	Lab 3: PyMol Viewer	100 pts
22	Lab 4: Fold-It Game (Rosetta based)	50 pts
29	Lab 5: Fold-It Game (Rosetta based)	100 pts
Oct 6	Lab 6: Evolutionary Sequence Variation with JalView	50 pts
13	Lab 7: Protein Modeling with PyRosetta	100 pts
20	Lab 8: Writing Python Scripts for PyRosetta	100 pts
27	Lab 9: Scoring to Evaluate Models	50 pts
Nov 3	<i>Student Holiday – Election Day</i>	
10	Lab 10: <i>de Novo</i> Protein Folding	100 pts
17	Lab 11: Structure Refinement	100 pts
24	<i>Thanksgiving Break</i>	
Dec 1	Lab 12: Protein Design in Rosetta	100 pts

*Last day to change registration is **August 25, 2020***

*Last day to drop the course with a **W** grade is **October 26, 2020***

*- after that date, any withdrawals receive a **WF** grade*